

HYDROGENOLYSIS OF DILUTE SOLUTIONS OF DIBENZYL IN TOLUENE AT COAL LIQUEFACTION CONDITIONS. Lonnie W. Vernon, Exxon Research and Engineering Company, P. O. Box 4255, Baytown, Texas 77520, and Ralph Livingston and Henry Zeldes, Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830.

Previous pyrolysis studies (L. W. Vernon, Fuel 59 102 (1980)) have shown that the conversion of dibenzyl in the presence of both tetralin and molecular hydrogen or in the presence hydrogen alone proceeds along two parallel reaction paths. Toluene is produced by a thermolysis reaction in which the rate controlling step is the thermal cleavage of the β -bond in dibenzyl. Benzene and ethyl benzene are produced by a hydrogenolysis reaction. The hydrogenolysis reaction is thought to proceed via a hydrogen atom chain carrier. ESR studies (R. Livingston, H. Zeldes, and M. S. Conradi, J. Amer. Chem. Soc. 101 4312 (1979)) have shown that benzyl is the predominant radical in the system during the pyrolysis of dilute solutions of dibenzyl in toluene. In the present study dilute solutions of dibenzyl in toluene have been pyrolyzed at 450°C, contact times of 1-3 minutes, and hydrogen pressures of 0-15 MPa. Under these conditions the conversion of dibenzyl is low (about 2-7%). The major product is benzene and the concentration of benzene increases with increasing hydrogen pressure. These results are consistent with the proposed mechanism for the conversion of dibenzyl in the presence of molecular hydrogen. In the present study, the free radical reaction is initiated by the thermolysis of dibenzyl and the benzene is produced by the hydrogenolysis of toluene via a hydrogen atom carrier.